Nonlinear Combustion Instability in

Liquid-Propellant Rocket Motors

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Introduction

This report describes the activities of MAGI during the first quarter of the present contract with the Jet Propulsion Laboratories. The report is written in several sections so that there will be clear delineation between topics. In section I the nonlinear fluid dynamic equations are presented as well as some comments on the reason for choosing this particular form for the integration process. Section II contains the complete theory for the linearized solution of a rotating transverse wave in a circular chamber. The equations are derived by usual perturbation techniques from the equations of Section I. Some results are graphically shown via computer generated plots. The evaporation and combustion model that will be coupled to the gas dynamic equations are presented in detail in Section III. The theory has the feature that ignition-extinction phenomena can be included. Section IV contains a short description of some sub-projects that are in various stages of completion. Included in this section is a short description of alternate procedures to be tested in the hydrodynamic portion of computer program COMB.

I. Fluid Dynamic Model - Nonlinear Differential and Difference Equations

The differential equations describing the motion of a compressible fluid in cylindrical coordinates can be written in vector form as

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial r} + \frac{\partial G}{\partial \theta} + \frac{\partial H}{\partial z} + S = \psi \tag{1}$$

The source term, ψ, has four components corresponding to the rate of production of mass, momentum and energy per unit volume. In section III, we show how to compute this vector. The vector W correspond to the mass, momentum in the r and θ directions and total energy, all per unit volume. The vectors F, G and H represent the flux of these quantities in the radial, tangential and axial directions respectively. It has been assumed that only four components are necessary in the representation of W, i.e., the axial component of momentum is ignored.

In order to compute the time dependent behavior of

$$W = r \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho(e + \tfrac{1}{2}(u^2 + v^2)) \end{pmatrix} \tag{2}$$

the fluxes

$$F = r \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E+p)u \end{pmatrix}, \quad G = \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ (E+p)v \end{pmatrix}, \quad H = r \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ (E=p)w \end{pmatrix} \tag{3}$$

must be known. The pressure is p, the total energy is E (the fourth component of W). The velocity components in the radial,

tangential and axial directions are u, v and w respectively. The vector S is obtained as a result of the transformation to cylindrical coordinates from cartesian coordinates and is given by

$$S = \begin{pmatrix} 0 \\ -(p+\rho v^2) \\ \rho uv \\ 0 \end{pmatrix} \qquad (4)$$

The components of ψ are schematically

$$\psi = \begin{pmatrix} \dot{\psi}(\rho) \\ 0 \\ 0 \\ \dot{\psi}(E) \end{pmatrix} \qquad (5)$$

The first and fourth terms correspond to the rate of generation of mass and energy per unit volume due to combustion. One observes that the sources of momentum generation have been set equal to zero. The contribution of such terms will be included in the future when some facility has been achieved with the present model.

Once the source term ψ is computer, then $\partial W/\partial t$ can be obtained if an approximation to the axial gradient can be computed. Since we are limiting the calculation to the transverse plane and time (rather than include a true three dimensional model by allowing z variations) an additional relation must be introduced in place of the time dependent axial momentum equation

$$(r\rho w)_t + (r\rho wu)_r + (\rho wv)_\theta + (r(p+\rho w^2))_z = 0 \qquad (6)$$

We emphasize this point because $\psi(t)$ 0 implies that the left hand side of (1) will be positive; hence, unless the axial (z) compo-

nent of flux is included in the model, the solution vector W will increase continually. If the calculation is to be carried out to arbitrary time, the accumulation can become arbitrarily large. It is certainly possible, in the complete three dimensional problem, for local accumulation to exist. However, it would require a three dimensional-time dependent calculation to ascertain the relative inaccuracy of the assumption

$$\frac{\partial}{\partial t} \iint W r dr d\theta = 0 \tag{7}$$

This relation allows an explicit calculation of $\partial H/\partial z$ at time t by using

$$\frac{\overline{\partial H}}{\partial z} = -\iint \{\frac{\partial F}{\partial r} + \frac{\partial G}{\partial \theta} + S - \psi\} \, r dr d\theta / \iint r dr d\theta \tag{8}$$

The bar over the axial derivative of the flux indicates that it is an average value used throughout the chamber cross section, i.e.,

$$\frac{\overline{\partial H}}{\partial z} = \overline{H}_z (t) \text{ only.}$$

Then equation (1) is written as

$$\text{div } (W, F, G, S) = \psi - \frac{\overline{\partial H}}{\partial z} \tag{9}$$

$$\text{div} = (\partial_t, \partial_r, \partial_\theta, 1)$$

The right member of equation (9) is then considered as specified.

The solution to our problem then lies on the making of suitable difference approximations to the left member of equation (9). The difference equations that are used in the approximation to equation (9) are of second order accuracy. If v represents a vector solution of the numerical problem, then v is defined on a

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lattice of net points r_i, θ_j which are defined as the intersection of lines of constant r and θ on the $r\text{-}\theta$ plane; then

$$\bar{v} = v(r_i, \theta_j, t + \tfrac{1}{2}\Delta t)$$

$$v(r_i, \theta_j, t+\Delta t) = v(r_i, \theta_j, t) - \frac{\Delta t}{r} \{ F_r(\bar{v}) + G_\theta(\bar{v})$$

$$+ S(\bar{v}) + \bar{H}_z - \psi(\bar{v}) \}$$

(10)

are the difference approximations which are accurate to $o(\Delta t^3)$, i.e., $\bar{v}$ itself satisfies

$$|\bar{v} - W| = \theta(\Delta t^2)$$

while

$$|v - W| = \theta(\Delta t^3)$$

Furthermore system (10) is stable in the sense of linear stability theory if

$$\frac{\Delta t}{\Delta} < \frac{1}{\sqrt{2}} \cdot \frac{1}{|u|+a}$$

The sound speed is a and the particle velocity is u while Δ is the space step. This result was first obtained by Richtmyer and has been born out in practical calculations. The exact form of equation (10) is given in Reference 20.

It is interesting to note that the difference equation used (equation (10)) is the analogue of the physical conservation laws so that, when numerical integration is performed with these difference equations, the result is the analogue of the integral equations. This means that across lines of discontinuity, the integral equation i.e., the Rankine-Hygoniot condition, will automatically be satisfied. Other forms of the conservation laws will in general not yield the proper jump conditions.

To see the relevance of these last remarks, consider a model equation of equation (1),

$$u_t + (F(u))_r = 0 \tag{11}$$

Let

$$F(u) = \tfrac{1}{2}u^2,$$

then the equation is nonlinear and discontinuities will develop in a finite time even if the initial data is smooth. Let $[p]$ signify the jump in the function p, then if these are lines of discontinuity in the solution to equation (11), the jumps must satisfy

$$S[u] = -\tfrac{1}{2}\left[u^2\right] \tag{12}$$

The normal speed of propagation of the discontinuity is given the symbol S. Now, however, multiply equation (11) by u and use the definition of $F(u)$. The resulting equation is

$$(\tfrac{1}{2}u^2)_t + (1/3u^3)_r = 0 \tag{13}$$

Hence discontinuities arising in the solution of equation (13) must have jumps in the solution u which satisfy

$$S\left[u^2\right] = -\left[\tfrac{2}{3}u^3\right] \tag{14}$$

It is clear then, that the strength of the discontinuity, if measured by say the jump in u, will, in general differ. The value of the jump will be a function of the form of the differential equation that is solved. Another example can be obtained immediately from equation (11), i.e., carry out the differentiation that is indicated in equation (11) and divide by u to obtain

$$(\ln u)_t + u_r = 0$$

which obviously has an associated jump condition which differs
from equation (12).

II.   <u>Linear Theory</u> - Transverse Rotating Wave

In this section we show that by neglecting the right member

of equation (9) the resulting system

$$W_t + F_r + G + S = 0 \qquad (1)$$

can be linearized and an exact solution in the domain $\mathcal{D}$ (which we

take as the unit disc) will be found. First we write system (1)

in its component form; by substracting the first component, i.e.,

the continuity equation, premultiplied by the $r(\theta)$ component of

velocity from the $r(\theta)$ momentum equation, one obtains the con-

tinuity equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \underline{q} = 0 \qquad (2a)$$

and the two momentum equations in the form

$$\frac{D\underline{q}}{Dt} = -\frac{1}{\rho r} \operatorname{grad} p + \frac{1}{\rho r} \begin{cases} p + \rho v^2 \\ -\rho uv \end{cases} \qquad (2b)$$

where $\frac{D}{Dt} \equiv (\ )_t + (\ )_r + \frac{v}{r}(\ )_\theta$ is the particle derivative in

polar coordinates and $\nabla \cdot \underline{q} \equiv (ru)_r + \frac{1}{r} v_\theta$ is the divergence in

these coordinates.

In the absence of irreversible changes (heat conduction,

viscous effects, etc.) the fluid undergoes a reversible adiabatic

change. The initial state of a fluid can be connected to its

final state through

$$p\rho^{-\gamma} = \text{constant for a particle} \qquad (3)$$

If the fluid is initially uniform the constant in equation (3) is

the same for each particle in the domain $\mathcal{D}$ It is then possible

to replace $D\rho$ by $a^{-2}Dp$, where a is the sound speed: and we do so

in system (2). Now, linearization is imposed so that a solution

of the linearized form of (2) can be obtained. Let $\rho = \rho_\infty + \rho^1$,

$p = p_\infty + p^1$ and $a_\infty = \gamma\, p_\infty/\rho_\infty$; then system (2) can be given in the linearized form

$$q_t = -\frac{1}{\rho_\infty r}\ \text{grad } p^1$$

$$p_t^1 = -\rho_\infty\, a_\infty^2\ \text{div } q$$

Here $q = \begin{pmatrix} u \\ v \end{pmatrix}$ is the fluid velocity which is the deviation from the initial uniform constant state. The term in the brackets of (2) can be neglected after linearization because it is quadratic in the velocity components. Now it is clear that since the vector q is given as the gradient of a scalar function, i.e., p^1, (also $\nabla \times q = 0$ because the entropy is constant) then the existence of a potential ψ is implied such that $q = \text{grad } \psi$, i.e., the components of q are given by

$$q = \begin{pmatrix} \psi_r \\ \frac{1}{r}\,\psi_\theta \end{pmatrix}$$

since the gradient operator is

$$\nabla (r,\theta) = \left(\frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial \theta} \right)$$

whence

$$\psi_t = -\rho_\infty^{-1} p^1 \quad \text{or} \quad \psi_{tt} = -\rho_\infty^{-1} p_t^1 \tag{5}$$

and $\qquad p_t^1 = -\rho_\infty\, a_\infty^2\, \nabla^2 \psi$

Then the wave equation can be obtained from the above basic equations of acoustic theory. The result is, of course, the **familiar** form $\qquad \psi_{tt} = a_\infty^2 \nabla^2 \psi \tag{6}$

In acoustic theory one usually expresses the solution of equation (6) as a series each term of which corresponds to a particular Fourier component. Once can also represent the solution of equation (6) as a sum of two solutions, i.e., ingoing and outgoing waves

$$\psi = g_1 (\underset{\sim}{\alpha} \cdot \underset{\sim}{x} - a_\infty t) + g_2 (\underset{\sim}{\alpha} \cdot \underset{\sim}{x} + a_\infty t) \tag{7}$$

where the plane waves travel at normal speed a_∞ in the α direction in the space of $\mathcal{D}(x)$. Since (6) is linear, the solution can be built up by a superposition of many of these waves given by equation (7).

Solutions to equation (6) can be most easily obtained by separation of variables. Since

$$\psi_{tt} = a_\infty^2 \ (\psi_{rr} + \frac{1}{r} \psi_r + \frac{1}{r^2} \psi_{\theta\theta}) \tag{8}$$

and the homogeneous boundary condition

$$\psi_r (1,\theta,t) = 0 \tag{9}$$

which expresses the fact that the normal velocity is zero at the boundary $r = 1$. Since we consider $\mathcal{D}$ to be the unit disc, normalization will be required when the radial component of the solution is generated. The initial conditions also have to be specified; they are

$$\psi(r,\theta,0) = \psi_0(r,\theta) = 0$$

and

$$\psi_t (r,\theta,t) \big|_{t=0} = - \rho_\infty^{-1} p^1 (r,\theta,0) \tag{10}$$

If we assume a solution of equation (8) of the form

$$\psi = R(r) \ \textcircled{H} \ (\theta) \ e^{\pm iKa_\infty t}$$

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Then the two ordinary differential equations for which R and $\textcircled{H}$ must satisfy are

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + (K^2-\frac{n^2}{r^2})\ R=0 \qquad (11)$$

$$\frac{d^2\ \textcircled{H}}{d\theta^2} + n^2\ \textcircled{H} = 0 \qquad (12)$$

To obtain the periodicity of ψ, that is $\psi(\theta+2\pi) = \psi(\theta)$, we restrict the numbers which **n** can take on to be integers. Hence $\textcircled{H}$ satisfies

$$\textcircled{H} = \ell^{\pm in\theta}$$

and for solutions which are finite at r=0 we have

$$R = J_n(Kr)$$

Here $J_n(Kr)$ denotes the Bessel function of the first kind of order and argument Kr. In such a manner solutions of equation (8) can be built up from a series which has terms of the form

$$J_n(Kr)^{\pm in\theta \pm iKa_\infty t}$$

To satisfy boundary condition (9) we set $J_n^{J'}(KR) = 0$, which is a transendental equation defining the numbers K(for n=1, $K \sim \frac{1.841}{R}$). We take the imaginary component of the above solution which leads to the traveling wave solution with n = 1.

$$\psi = \varepsilon J_r(Kr)\ \sin\ (Ka_\infty t+\theta)$$
$$p^1 = \gamma p_\infty K\varepsilon\ J\ (Kr)\ \cos\ (Ka_\infty t+\theta) \qquad (13)$$

It is clear that the above result is of the same form as given by equation (7). The density is computed using equation (3) and ε is a dimensionless measure of the amplitude defined below.

The solution we seek of equation (8), i.e., equation (13) will satisfy the boundary condition of zero normal velocity at r = R. In addition the solution will also satisfy the initial conditions given by equation (10) if we take

$$\psi_0 = \epsilon J_n(Kr) \sin n\theta$$

and

$$\partial\psi/\partial t = -\epsilon a_\infty K J_n(Kr) \cos n\theta \quad , \quad n = 1$$

to be the initial data.

Finally, one observation: The solution is completely obtained with the specification of only one boundary condition, i,e, $u(R,t) = 0 = \partial\psi/\partial r$. This result is carried over to the nonlinear problem.

System (13) has been programmed and incorporated into program COMB (Reference 20) as initial data. Since the solution represented by system (13) is physically the deviation from the uniform state, we can define a dimensionless parameter measuring the max of this deviation $p^1{}_{max} = p^*$:

$$\epsilon = \frac{(p_\infty + p^*) - p_\infty}{\gamma p_\infty J_1(K^*)} = p^*/(p_\infty \gamma J_1(K^*)) \quad , \quad K^* = 1.841...$$

which essentially measures the deviation from uniformity at the point $(r,\theta,t) = (R_{max}, 0, 0)$. The solution is then parametized in terms of ϵ, i.e., the pressure at any point on the disc is

$$p(r,\theta,t)/p_\infty = 1 + \epsilon\gamma J_1(K^*)$$

The solution for the pressure is given in Figure (1) for t = 0. For t>0 the contour lines (isobars) undergo a uniform rotation corresponding to a spinning mode. The plot of the density field

is similar. Figure (2) and Figure (3) correspond to lines of constant $\partial\psi/\partial r$ and $\frac{1}{r}\partial\psi/\partial\theta$ respectively:

$$\frac{u}{a_\infty} = \epsilon J_1'(Kr)\,\sin(Ka_\infty t+\theta), \quad J_1' \equiv \frac{1}{2}(J_0 - J_2)$$

$$\frac{v}{a_\infty} = \frac{\epsilon J(Kr)}{(\frac{K^*}{R} r)}\,\cos(ka_\infty t+\theta)$$

The singularity at $r = 0$ offers no difficulty since the identity

$$\frac{J_n(x)}{x} = \frac{1}{2n}\left(J_{n-1}(x) + J_{n+1}(x) \right)$$

shows that v/a_∞ is well behaved for all x in $\mathcal{B}$.

THE DROPLET EVAPORATION AND COMBUSTION ANALYSIS

III. The "Complete" Model (Computation of ψ)

Initially, the propellant system will be taken to be hydrazine (N_2H_4)/nitrogen tetroxide (N_2O_4). The oxidation behavior of this system has been the subject of intensive investigation for a number of years (Ref. 1 through 10). Recent evidence (Ref. 10) suggests that at moderate pressures, hydrazine decomposition occurs very close to the droplet surface, with the combustible decomposition products (NH_3 and H_2) partially oxidizing first with NO, followed by complete oxidation with O_2. The two distinct oxidation regimes result in the two-flame appearance characteristic of N_2H_4/N_2O_4 droplet combustion.

Since the rate-controlling chemical kinetic reactions are likely to change under very low or very high pressure conditions (the former is characteristic of high-altitude ignition, and the latter of high pressure rocket motor operation), a complete model of hydrazine droplet combustion would be one which includes a detailed description of the chemical kinetics. If it is assumed initially that the droplet undergoes spherically-symmetric, quasi-steady-state burning at constant pressure in quiescent oxidizer surroundings, and if it is further assumed that no viscous or body forces are present, and that thermal radiation can be neglected, the three-dimensional, time-dependent spherical conservation equations can be shown to reduce to:

1. Overall Continuity

$$\frac{d}{dr} (\rho r^2 v) = 0 \qquad (1)$$

which if integrated between the droplet surface
and any arbitrary radial location becomes

$$\rho v r^2 = \rho_s v_s r_D^2 \qquad (2)$$

2. Species Continuity

$$\frac{1}{r^2}\left(ar_D \frac{dY_i}{dr} - \frac{d}{dr}\left(r^2 \frac{dY_i}{dr}\right)\right) = \frac{Sc}{\mu} R_i \qquad (3)$$

where a is a dimensionless mass burning rate:

$$a \equiv \frac{\rho_s v_s r_D}{\rho D} \qquad (4)$$

Y_i = mass fraction of species i,

Sc = dimensionless Schmidt number ($\mu/\rho D$),

R_i = rate of generation or disappearance of i,

D = the diffusion coefficient

The boundary conditions for equation (3) are that (a) the
net mass flux of all species (excepting the fuel, N_2H_4) at the
droplet surface must equal zero:

$$\text{at } r = r_D: \quad \frac{a}{r_D} Y_i = \frac{dY_i}{dr} \; ; \; i \neq N_2H_4 \qquad (3a)$$

$$\frac{a}{r_D}(Y_i - 1) = \frac{dY_i}{dr} \; ; \quad i = N_2H_4$$

and (b) as $r \to \infty$, the gas environment consists only of N_2O_4 and its
decomposition products (NO_2, NO, and O_2):

$$\text{as } r \to \infty: \quad Y_i = 0; \; i = 1, 2, 3, 4 \qquad (3b)$$

$$Y_i = Y_{i,\infty} \; ; \; i = 5, 6, 7, 8$$

The species numbering system is indicated in Table I.
If the N_2O_4 and its products are assumed to be in chemical equili-
brium, the $Y_{i,\infty}$ values are readily calculated.

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3. Energy Conservation

$$\frac{1}{r^2} \left(ar_D c_p \frac{dT}{dr} - \frac{1}{Le} \cdot \frac{d}{dr} \left(r^2 c_p \frac{dT}{dr} \right) \right) =$$

$$\frac{dT}{dr} \left(\sum_i c_{p_i} \frac{dY_i}{dr} \right) - \frac{Sc}{\mu} \cdot \sum_i H_i R_i \qquad (5)$$

where Le = Lewis number $(\rho D c_p / k)$

    k = thermal conductivity

    c_p = mixture specific heat $(\sum_i Y_i c_{p_i})$

    H_i = enthalpy of species i

The appropriate boundary conditions are that (a) when the temperature of the droplet is taken to be uniform and constant, the heat conducted to the droplet must equal the heat required to vaporize the fuel leaving the droplet:

at $r = r_D$: $\frac{1}{Le} \left(c_p \frac{dT}{dr} \right) = \frac{a}{r_D} L$ (5a)

and (b) as $r \rightarrow \infty$, the temperature approaches the rocket environmental temperature:

as $r \rightarrow \infty$: $T \rightarrow T_\infty$ (5b)

A series of species generation equations are required (the R_i terms). The actual chemical kinetic mechanism for N_2H_4/N_2O_4 is known to be enormously complicated, involving tens of species and probably well over one hundred elementary chemical reactions (Ref. 11). As an initial approximation to the actual chemical kinetic mechanism, the sequence of ten overall (global) irreversible reactions shown in Table II may be taken to represent the kinetic mechanism. Sawyer (Ref. 6) has investigated each of these reactions, and his values for the individual reaction rate constants are given in Table II. (It should be noted that Sawyer observed no reaction between NH_3 and NO, and between H_2 and NO,

which reduces this kinetic mechanism to 8 overall, irreversible reactions.) Based on this kinetic mechanism, the R_i terms may be written in terms of the reaction rate constants (k_m), the gas density, and the species mass fractions and molecular weights as shown in Table III.

Assuming all gases to be ideal, the equation of state may be written

$$\rho = \frac{P}{R_o T \sum\limits_{i} \frac{Y_i}{M_i}} \tag{6}$$

Given the required thermochemical data $(c_{p_i}, H_i, \text{etc.})$, equations (1), (3), (5), (6) and the R_i equations (Table III), with the associated boundary conditions lead to an equation system in which a number of parameters must take on particular values; that is, this formulation leads to a multiple eigenvalue problem. The physical necessity for multiple eigenvalues in a subject of current research and debate (References 12 though 16). Wehner (Ref. 16) argues that the second eigenvalue may be a kinetic parameter to which the flammability limits are related. (The first eigenvalue is the flame velocity in the theory of laminar, one-dimensional, premixed flames, and is the surface mass flux, $_s v_s$, in the droplet flame problem.) Williams (Ref. 15) refutes Wehner's arguments for the existence of more than one physical eigenvalue. In any event, the work of Campbell (References 12 through 14) indicates the current inability to obtain solutions to system of equations of this type without a number of additional simplifying assumptions.

THE MODIFIED FLAME SURFACE ANALYSIS

Recently, Peskin (References 17 and 18) has obtained solutions to the problem of a fuel droplet burning steadily in an oxidizing atmosphere by assuming, in addition to the assumptions noted in the previous section, that the reaction mechanism could be adequately represented by a one-step, irreversible reaction of the type:

$$\nu_F F + \nu_o O \xrightarrow{k_f} \nu_p P \tag{7}$$

where the ν_i represent the stoichiometric coefficients, F is the fuel, O the oxidizer, and P the product; (b) assuming the Lewis number to be unity; (c) taking constant averaged values for the specific heats, density, and heats of vaporization and combustion; (d) assuming transport parameters independent of temperatures and chemical composition; (e) neglecting the energy transport due to species diffusion (i.e., the term $\dfrac{dT}{dr}\left(\sum\limits_i c_{p_i} \dfrac{dY_i}{dr}\right)$ in equation (5)); (f) and by employing the modified flame surface approximation discussed below.

Although the analysis employs a number of assumptions, it has the advantage of retaining some aspect of the chemical kinetics. As a result, the feature of droplet extinction and re-ignition is retained, one which is of potential consequence in an unstable rocket system wherein the droplets may encounter regions of expansion and compression. Since droplet combustion analyses which assume diffusional processes to be rate-controlling neglect the chemical kinetics entirely, the extinction-ignition feature is absent. Such an approximation is discussed in the next section.

Employing the additional assumptions discussed above, the species continuity equation

$$\frac{1}{r^2}\left(ar_D\frac{dY_i}{dr} - \frac{d}{dr}\left(r^2\frac{dY_i}{dr}\right)\right) = \frac{R_i}{\rho D}$$

may be written

$$a\frac{dY_i}{d\eta} - \frac{d}{d\eta}\left(\eta^2\frac{dY_i}{d\eta}\right) = i_i\ \eta^2 b\left(\frac{M_F^{1-N_F}}{M_O^{N_O}}\right)\left[Y_F\right]^{N_F}\left[Y_O\right]^{N_O} \qquad (8)$$

where $\eta \equiv \frac{r}{r_D}$, $b \equiv \frac{r_D^2 B}{D}$, $B \equiv \rho A(T)e^{-E/R_OT}$, and N_F and N_O represent the reaction orders with respect to fuel and oxidizer. The i_i term arises from the fact that $R_{ox} = \frac{\nu_O M_O}{\nu_F M_F}R_F$ and $R_p = -\frac{\nu_P M_P}{\nu_F M_F}R_F$. Thus, for the assumed one-step, irreversible reaction

$$N_2H_4 + NO_2 \rightarrow 2\ H_2O + \frac{3}{2}\ N_2 \qquad (9)$$
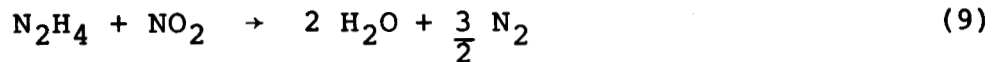
$i_1 = -1$, $i_2 = -(23/16)$, $i_3 = (9/8)$, and $i_4 = (21/16)$.

The simplified form of the energy equation (equation 5) is

$$\frac{1}{r^2}\left(ar_D\frac{d}{dr}(c_pT) - \frac{d}{dr}\left(r^2\frac{d}{dr}(c_pT)\right)\right) = \frac{-1}{\rho D}\sum_i H_iR_i \qquad (10)$$

Introducing the notation $t \equiv (T-T_\infty)/(Q/c_p)$, and $Q = H_1+i_2H_2+i_3H_3+i_4H_4$, equation (10) becomes:

$$a\frac{dt}{d\eta} - \frac{d}{d\eta}\left(\eta^2\frac{dt}{d\eta}\right) = \eta^2 b\left(\frac{M_F^{1-N_F}}{M_O^{N_O}}\right)\left[Y_F\right]^{N_F}\left[Y_O\right]^{N_O} \qquad (11)$$

Writing equation (9) for the fuel, multiplying the resulting expression by i_2, then subtracting from it equation (9) written for the oxidizer, leads to:

$$a\frac{d}{d\eta}\left(i_2Y_F-Y_O\right) - \frac{d}{d\eta}\left(\eta^2\frac{d}{d\eta}\left(i_2Y_F-Y_O\right)\right) = 0 \qquad (12)$$

which can be integrated to yield:

$$i_2Y_F-Y_O = c_1+c_2\ \exp\ (-a/\eta) \qquad (13)$$

Subtracting equation (9) for the fuel from equation (11) leads to:

$$a\frac{d}{d\eta}(t+Y_F) - \frac{d}{d\eta}\left(\eta^2\frac{d}{d\eta}(t+Y_F)\right) = 0 \tag{14}$$

which, when integrated, becomes:

$$Y_F + t = c_3 + c_4 \exp(-a/\eta) \tag{15}$$

The boundary conditions equations (3a), (3b), (5a) and (5b) reduct to

at $\eta=1$:

$$\left.\frac{d}{d\eta}Y_k\right|_{\eta=1} = aY_k\Big|_{\eta=1}; \quad k = O,P$$

$$\left.\frac{d}{d\eta}Y_F\right|_{\eta=1} = aY_F\Big|_{\eta=1} - a \tag{12a}$$

as $\eta\to\infty$:

$$Y_F\Big|_{\eta\to\infty} = 0$$

$$Y_k\Big|_{\eta\to\infty} = Y_{k,\infty}; \quad k = O,P \tag{12b}$$

at $\eta=1$:

$$\left.\frac{dt}{d\eta}\right|_{\eta=1} = \frac{L}{Q}a \tag{14a}$$

as $\eta\to\infty$:

$$t\Big|_{\eta\to\infty} = 0$$

Insertion of the appropriate boundary conditions into equation (15), and after algebraic manipulation, an expression can be derived for the dimensionless mass burning rate:

$$a = \ln\left(\frac{1 + t_s - \frac{L}{Q}}{1 - Y_{F,s} - \frac{L}{Q}}\right) \tag{16}$$

where $t_s = t\Big|_{\eta=1}$ and $Y_{F,s} = Y_F\Big|_{\eta=1}$.

The analysis, which is currently in progress for the N_2H_4/NO_2 system, next assumes that a flame surface is located at $\eta = \eta^*$ where the fuel-oxidant ratio is stoichiometric. The reaction rate terms

on the right-hand sides of equations (9) and (11) are replaced by Dirac-delta functions; e.g., for the fuel, equation (9) becomes

$$a\frac{dY_F}{d\eta} - \frac{d}{d\eta}\left(\eta^2 \frac{dY_F}{d\eta}\right) = -\eta^2 b i_o N_o Y_F^* {}^{(N_F+N_o)} \delta(\eta-\eta^*) \qquad (17)$$

where $Y_F^* = Y_F\big|_{\eta=\eta^*}$ and $\delta(\eta)$ is the delta-function.

Equation (17) can be integrated using generalized function theory to yield an expression for the fuel distribution:

$$Y_F = \frac{b^*}{a} i_o N_o Y_F^* {}^{(N_o+N_F)} \eta^{*2} e^{-a/\eta} \begin{Bmatrix} 1-e^{a/\eta} & \text{for } \eta > \eta^* \\ 1-e^{a/\eta^*} & \text{for } \eta \le \eta^* \end{Bmatrix} + 1-e^{-a/\eta} \qquad (18)$$

Similar expressions can be derived for the oxidizer, product, and temperature distributions.

One key aspect of the above analysis is that a satisfactory overall reaction rate constant (i.e., B) be inserted into the above analysis in order to obtain a realistic representation of the "actual" chemical kinetics over a wide range of operating conditions. Currently, the "complete" gas-phase chemical kinetic system detailed in Table II is being programmed into a one-dimensional analysis describing flow along a streamline. From the results obtained over a range of conditions, the appropriate values for A(T) and the activation energy, E, can be obtained for the hydrazine-NTO system for insertion into the above analysis.

THE DIFFUSION-CONTROLLED FLAME ANALYSIS

In an effort to test out the behavior of hydrodynamics code with and without chemical reactions, a diffusion flame model was developed. Introducing the rate of disappearance of the fuel

$$\dot{m}_F^o \equiv \rho_s v_s (4\pi r_D^2) \qquad (19)$$

Setting $Q = Q_T$, where Q_T is the heat of reaction per unit mass of fuel and oxidizer consumed, using the definition of t_s ($t_s = c_p(T_s - T)/Q$), and the fact that Le = 1, and noting that $Y_{F,s} = 1$ for this elementary diffusion flame model, equation (16) reduces to

$$\dot{m}_F^0 = \frac{4\pi r_D k}{c_p} \ln \left(1 + \frac{c_p(T_\infty - T_s) + Y_{O,\infty} \Phi f_s \Delta H_R}{L} \right) \tag{20}$$

where $Q_T = Y_{O,\infty} \Phi f_s \Delta H_R$, $Y_{O,\infty}$ is the mass fraction of oxidizer in the chamber gases, Φ is the fuel-oxidant equivalence ratio, f_s is the stoichiometric fuel-oxidant ratio, ΔH_R is the heat of reaction per unit mass of fuel, and the superscript zero on the $\dot{m}_F^0$ term indicates that this is the fuel mass flux in a __stationary__ environment; that is, in the absence of forced convection effects. Written in a slightly modified form, equation (20) is frequently referred to as the Godsave equation. As a first approximation, the mass flux dependence on the fact that there will, in general, be a difference in velocity between the droplet and its surroundings will be assumed to be given by the expression of Agoston, Wise, and Rosser (Reference 19):

$$\frac{\dot{m}_F}{\dot{m}_F^0} = 1 + 0.276 \ (\text{Re})^{\frac{1}{2}} \ (\text{Pr})^{\frac{1}{3}} \tag{21}$$

where $\text{Re} = (2\rho_\infty r_D) \ |u-v|/\mu_\infty$ and $\text{Pr} = c_{p\infty}\mu_\infty/k_\infty$.

In this manner, the components of the ψ-vector of the hydro-dynamics code can be written (assuming no drag force interactions for the pancake motor model):

$$\psi = \begin{pmatrix} \dot{m}_F \ (1+\frac{1}{\Phi f_s}) \\ 0 \\ 0 \\ \dot{m}_F \ (\Delta H_R - L - \frac{L_O}{\Phi f_s}) \end{pmatrix} \qquad (22)$$

where L_O is the latent heat of the oxidizer. This elementary diffusion flame analysis is currently being coupled with the hydro-dynamics code.

IV. Program COMB Status

This past quarter saw a rapid expansion of the basic computer program COMB. The major accomplishments are:

1. Incorporation of nine subroutines which constitute a graphical display package for use on Calcomp digital display devices. This basic package was obtained from another installation and required some extensive modification for use with COMB. Also, two additional subroutines were required which act as an interface between the numerical portion of the code and the graphical display package.

2. Incorporation of several subroutines which carry out numerical quadratures in two space dimensions in the r-θ plane. The theory behind these routines are given in Appendix A of this report. These routines carry out the execution of equation (8) of Section II.

3. A subroutine, to compute ψ given in equation (1) of Section I, was written and is presently being checked out. This subroutine incorporates all of the theory of Section IV and is essentially a computation of equation (22) of this section.

4. Generation of two subroutines used to compute the theory of Section II. These routines essentially generate the initial conditions of the fluid dynamic flow field corresponding to a spinning tangential wave of either finite or infinitesimal amplitude. The basic structure of these two routines were contained in a program listing communicated to us by Dr. George Sotter, for which we express our gratitude.

5. More accurate approximations have been constructed for calculation of special mesh points in COMB. The emphasis has been spent on boundary points and the center point calculation. The boundary point calculation is presently undergoing experimentation, the center point calculation has yet to be coded and tested.

6. The logic of COMB has been altered so as to include the source and flux terms as shown in equation (9), Section I.

We would like to give some details relating to statement 5 given above. First a few remarks on the specification of the boundary $r = R$. The linear theory shows that once $u(R,\theta,t) = 0$, is specified, the flow field is determined for all t. We write the corresponding boundary condition using the conservation of radial momentum

$$\frac{\partial \rho u r}{\partial t} = 0 = - \frac{\partial (\,(\rho u^2+p)r\,)}{\partial r} \quad - \frac{\partial \rho u v}{\partial \theta} \,+ (p+\rho v^2)$$

at a point on the boundary. Since $u = 0$, $(\rho u v)_\theta = 0$ and the difference approximation to the above relation at $(r_i,\ \theta_j)$ becomes

$$r(\rho u^2+p)_{i+\frac{1}{2},j+\frac{1}{2}} - r(\rho u^2+p)_{i-\frac{1}{2},j+\frac{1}{2}} + r(\rho u^2+p)_{i+\frac{1}{2},j-\frac{1}{2}}$$

$$- r(\rho u^2+p)_{i-\frac{1}{2},j-\frac{1}{2}} + r(\rho u^2+p)_{i+1,j} - r(\rho u^2+p)_{i-1,j}$$

$$= 2\Delta r \left(\frac{(p+\rho v^2)_{i+1,j} + (p+\rho v^2)_{i-1,j}}{2} \right) + \frac{\Delta r}{2} \left((\rho v^2+p)_{i+\frac{1}{2},j+\frac{1}{2}} \right.$$

$$\left. + (\rho v^2+p)_{i-\frac{1}{2},j+\frac{1}{2}} + (\rho v^2+p)_{i+\frac{1}{2},j-\frac{1}{2}} + (\rho v^2+p)_{i-\frac{1}{2},j-\frac{1}{2}} \right)$$

If the subscript + denotes image points then the subscript −
denotes the corresponding interior point and using

$$(\rho r)_+ = (\rho r)_-$$

$$u_+ = -u_-$$

$$(\rho v^2)_+ = (\rho v^2)_-$$

as reflection rules the condition

$$p_+ = p_- + \Delta r \left(\frac{\rho v^2}{R} \right)_-$$

will yield a zero value of normal velocity. The above condition
on the radial pressure gradient states that it is just balanced
by the centrifugal force $\rho v^2/R$ in the radial direction due to
fluid motion in the tangential direction. In cartesian coordinates
the above conditions reduce to the familiar forms $\rho_+ = \rho_-$, $u_+ = -u_-$,
$v_+ = v_-$ and $p_+ = p_-$.

The center point calculation is going to be modified from
the present method as stated in Reference 20. The new method
attempts to compute the divergence of the flow field at r = 0, i.e.,
$\partial W/\partial t$ is known if $\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}$
is known. Note that we use cartesian coordinates for this cal-
culation so that the x-y velocity components are related to the
r-θ velocity components through

x-component: $u = u_r \cos\theta - v_\theta \sin\theta$

y-component: $v = u_r \sin\theta + v_\theta \cos\theta$

We transform $f(r,\theta) \rightarrow f(x,y)$ and $g(r,\theta) \rightarrow g(x,y)$ using the above
transformation. The density and pressure are not effected by
coordinate transformations.

Now, if we consider a region R with boundary ∂R in the x-y plane then if ∂f/∂x, and ∂g/∂y exist, then

$$\frac{\partial f}{\partial x} = \oint_{\partial R} f dy \Big/ \oint_{\partial R} x dy$$

$$\frac{\partial g}{\partial y} = -\oint_{\partial R} g dx \Big/ \oint_{\partial R} x dy$$

and where all contour integrals are taken counterclockwise. For this calculation ∂R is a circle of radius Δr and the contour integrals are approximated by the sums

$$\widehat{\frac{\partial f}{\partial x}} \approx \sum_{j=1}^{N} (f_{j+1}+f_j)(y_{j+1}-y_j) \Big/ \sum_{j=1}^{N} (x_{j+1}+x_j)(y_{j+1}-y_j)$$

$$(1)$$

$$\widehat{\frac{\partial g}{\partial y}} \approx -\sum_{j=1}^{N} (g_{j+1}+g_j)(x_{j+1}-x_j) \Big/ \sum_{j=1}^{N} (x_{j+1}+x_j)(y_{j+1}-y_j)$$

Then

$$W(0,t+\Delta t) = W(0,t) - \Delta t \left(\widehat{\frac{\partial f}{\partial x}} + \widehat{\frac{\partial g}{\partial y}} \right) \qquad (2)$$

The values of f and g used in the sums in equation (1) are evaluated at t+Δt/2 so that equation (2) is second order accurate, consistent with regular mesh points in the interior of the combustion chamber.

PLOT OF PRESSURE P

FIGURE 1

PLOT OF U=M/RHO

FIGURE 2

29

PLOT OF V=N/RHO

NUMERICAL 5 PT BC

15 CONTOUR LEVELS

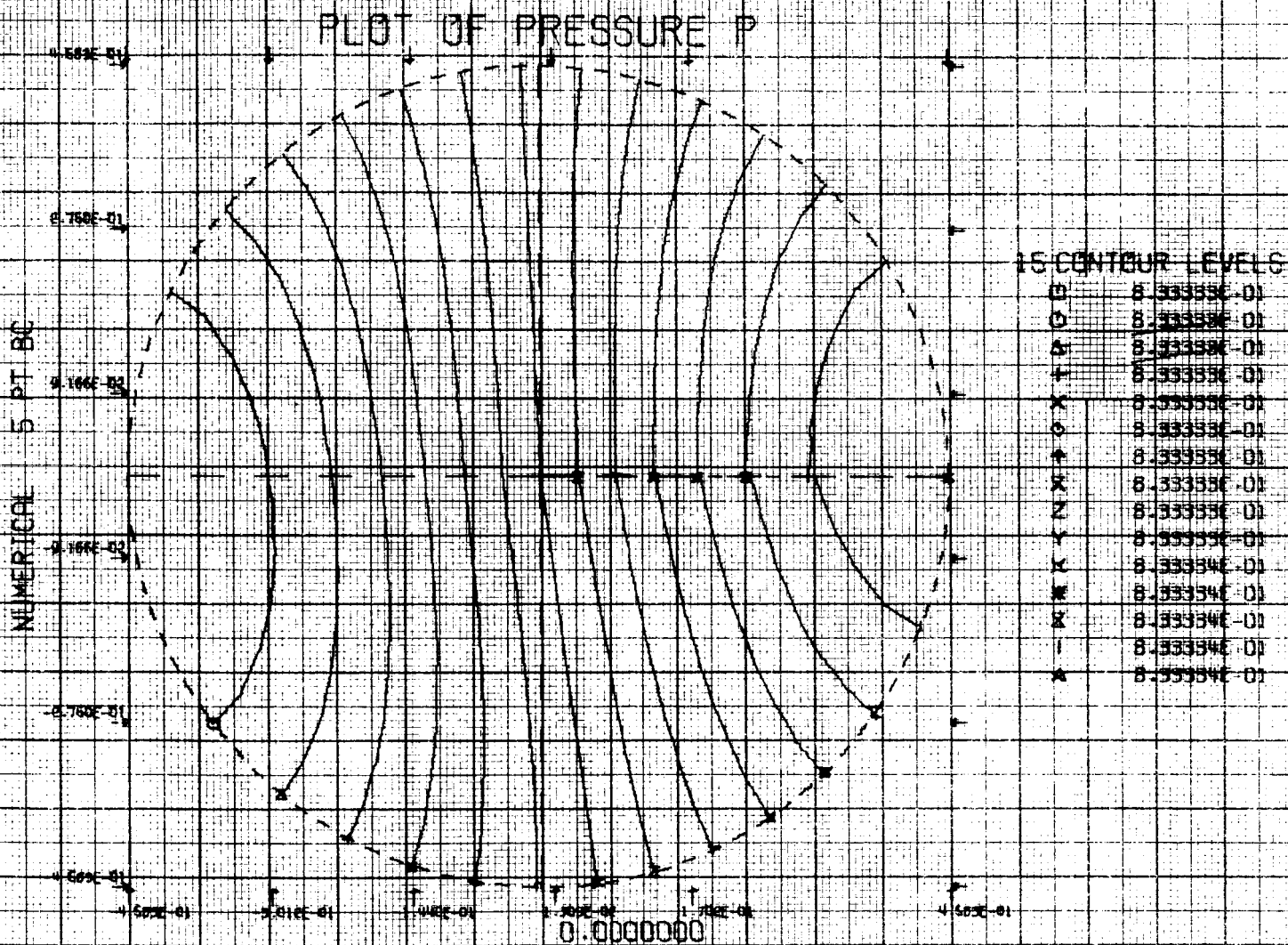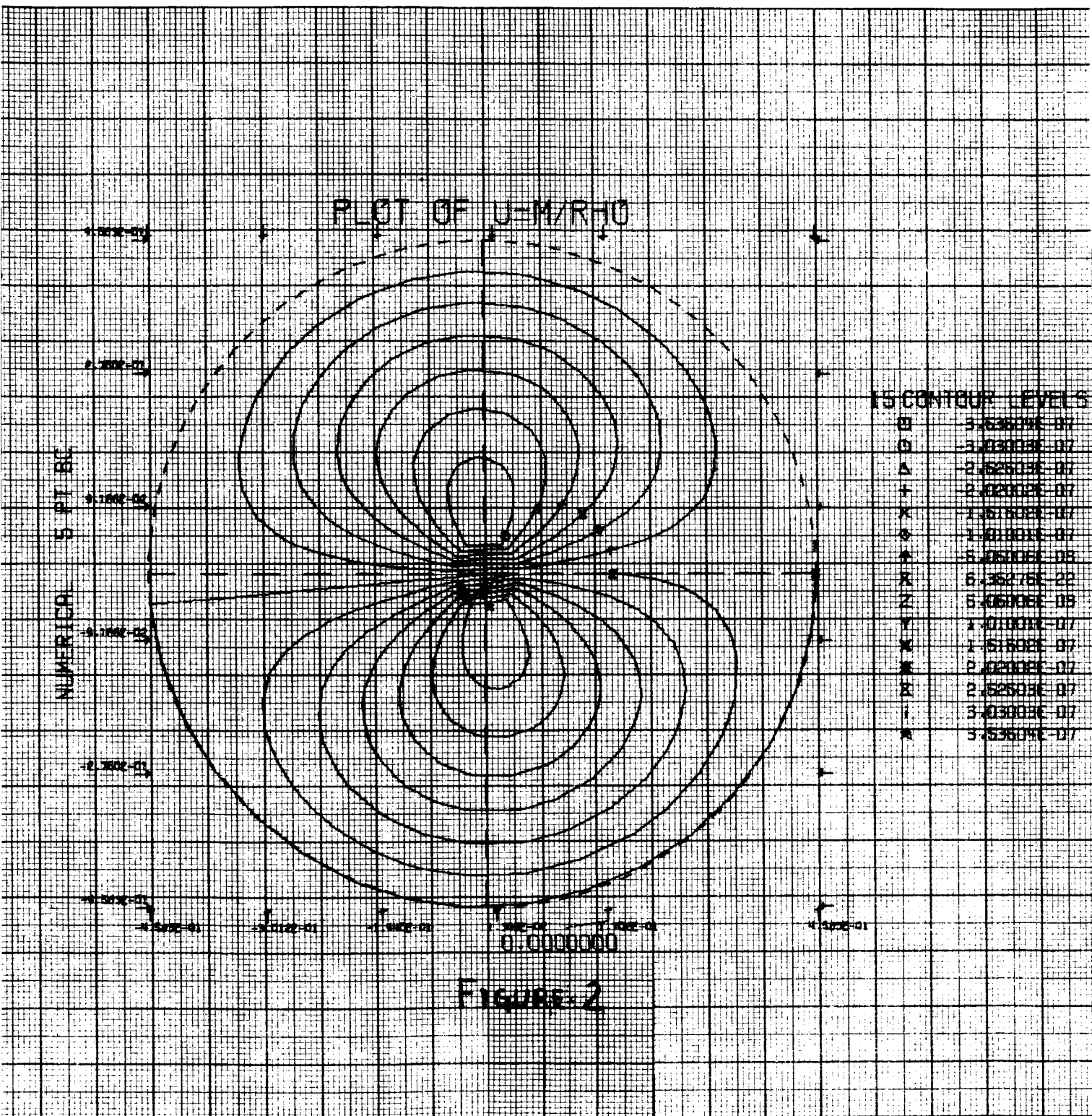|	
□	-3.56529E-07
○	-3.05596E-07
△	-2.54664E-07
+	-2.03731E-07
X	-1.52798E-07
◇	-1.01866E-07
✦	-5.09327E-08
⊠	3.17657E-21
Z	5.09327E-08
Y	1.01866E-07
X	1.52798E-07
W	2.03731E-07
V	2.54664E-07
⊣	3.05596E-07
★	3.56529E-07

0.0000000

FIGURE 3

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APPENDIX A

Consider Integrals of the form

$$I\{W\} = \int_0^R \int_0^{2\pi} W d\theta r dr$$

W is a vector valued function

$$W = W(r,\theta)$$

The domain of integration is defined for $0 \leq \theta \leq 2\pi$ and $0 \leq r \leq R$.

Introduce for the function W a function of the single variable r via

$$\beta(W;r) = \int_0^{2\pi} W(r,\theta) d\theta$$

Then the double integral becomes

$$I\{W\} = J\{\beta\} = \int_0^R \beta(W;r) r dr$$

In general the inteval $[0,R]$ will have N+1 net points that may be even. This does not allow the use of Simpsons rule since the number of points must be odd. For the case of even number of net points the following procedure may be used. Let h be the step size then

$$\int_0^R = \int_0^{3h} + \int_{3h}^R$$

where

$$\int_0^{3h} \beta(W;r) r dr = \frac{3h}{8} \left[3\beta'(W;h) + 3\beta'(W;2h) + \beta'(W;0) \right.$$

$$\left. + \beta'(W;3h) \right] + e_1, \quad \beta' = r\beta$$

$$e_1 = -\frac{3h^5}{80} \beta^{(IV)}(\xi) \quad 0 < \xi < 3h$$

and

$$\int_{3h}^{r} \beta(W;r)r\,dr = \frac{h}{3}\left[\beta'(W;3h) + \beta'(W;R) + 2\sum_{j=1}^{m-1}\beta(w;3h+2jh)\right.$$

$$\left. + 4\sum_{j=1}^{m-1}\beta(W;3h+(2j-1)h)\right] + e_2$$

$$e_2 \equiv \frac{R}{180}h^4\beta^{(IV)}{}_{(\xi)}$$

It remains for us to evaluate $\beta(W;r)$. A condition of periodicity exists on W, i.e.,

$$W(\theta+2\pi) = W(\theta)$$

The Euler-Maclaurin summation formula with $h=h_\theta$

$$\sum_{j=0}^{p-1} W(\theta+jh) = \frac{1}{h}\int_{\theta}^{\theta+ph} W(\tau)d\tau - \frac{1}{2}\left[W(\theta+ph)-W(\theta)\right]$$

$$+ \frac{h}{12}\left[W'(\theta+ph)-W'(\theta)\right] - \frac{h^3}{120}\left[W'''(\theta+ph)-W'''(\theta)\right]$$

$$+ \frac{h^5}{30240}\left[W^{IV}(\theta+ph) - W^{IV}(\theta)\right] - \cdots$$

letting $p=1$ and $\theta=0$

$$\int_0^h W(\tau)d\tau = hW(0) + \frac{h}{2}\left[W(h)-W(0)\right]$$

$$- \frac{(h)^2}{12}\left[W'(h)-W'(0)\right] + \cdots$$

The brackets cancel to zero if the above formula is used for all the intevals (θ_j, θ_{j+1}) $0<j<N-1$ in the interior for the function $W(\tau)$ and also at θ_0 and θ_N due to periodicity.

$$\beta(W;r) = \int_0^L W(r;\theta)d\theta = \frac{L}{N} \sum_{j=0}^{N-1} W(r, \theta_j) + e \qquad (*)$$

$$e = h^{2m+2} \, 2\pi C_m \, W^{(2m+2)}(\xi) \qquad \underline{o} < \xi \leq 2\pi$$

where $W \in C^{2m+2} \, [0, 2\pi]$ and is 2π periodic. This formulae, (*), is used in the integration routines in COMB.

TABLE I

SPECIES	MOLEC. WT.	HEAT OF FORMATION (kcal/mole)
1) N_2H_4	32	22.750
2) NH_3	17	-11.040
3) H_2	2	0
4) N_2	28	0
5) N_2O_4	92	2.170
6) NO_2	46	7.910
7) NO	30	21.580
8) O_2	32	0
9) H_2O	18	-57.798

TABLE II

REACTION	ORDER	REACTION RATE CONSTANT
1) $N_2H_4 \rightarrow NH_3 + \tfrac{1}{2}H_2 + \tfrac{1}{2}N_2$	1	$10^{10.33} \exp\left(-\dfrac{36,170}{RT}\right)$
2) $N_2H_4 + 4NO_2 \rightarrow 6NO + 2H_2O$	2	$10^{15.83} \exp\left(-\dfrac{26,700}{RT}\right)$
3) $N_2H_4 + 2NO \rightarrow 2H_2O + 2N_2$	1	$10^{10.17} \exp\left(-\dfrac{39,600}{RT}\right)$
4) $N_2H_4 + O_2 \rightarrow 2H_2O + N_2$	1	$10^{9.91} \exp\left(-\dfrac{37,200}{RT}\right)$
5) $NH_3 + \dfrac{5}{2}NO_2 \rightarrow \dfrac{7}{2}NO + \dfrac{3}{2}H_2O$	2	$10^{15.85} \exp\left(-\dfrac{33,800}{RT}\right)$
6) $NH_3 + 3NO \rightarrow \dfrac{5}{2}N_2 + \dfrac{3}{2}H_2O$	-	No Reaction
7) $NH_3 + \dfrac{3}{4}O_2 \rightarrow \dfrac{1}{2}N_2 + \dfrac{3}{2}H_2O$	2	$10^{14.61} \exp\left(-\dfrac{38,700}{RT}\right)$
8) $H_2 + NO_2 \rightarrow NO + H_2O$	2	$10^{21.5} \exp\left(-\dfrac{58,000}{RT}\right)$
9) $H_2 + NO \rightarrow H_2O + \tfrac{1}{2}N_2$	-	No Reaction
10) $H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$	1	$10^{10.96} \exp\left(-\dfrac{38,200}{RT}\right)$

· TABLE III

SPECIES GENERATION EQUATIONS

(a) $\quad R_1 = -\rho Y_1 \left(k_1 + k_2 \left(\dfrac{\rho Y_6}{M_6} \right) + k_3 + k_4 \right)$

(b) $\quad R_2 = k_1 \, \rho Y_1 \, \dfrac{M_2}{M_1} - \rho Y_2 \left(k_5 \dfrac{\rho Y_6}{M_6} + k_7 \dfrac{\rho Y_8}{M_8} \right)$

(c) $\quad R_3 = \tfrac{1}{2} k_1 \, \rho Y_1 \, \dfrac{M_3}{M_1} - \rho Y_3 \left(k_8 \dfrac{\rho Y_6}{M_6} + k_{10} \right)$

(d) $\quad R_6 = -\rho Y_6 \left(4 k_2 \, \dfrac{\rho Y_1}{M_1} + \dfrac{5}{2} k_5 \, \dfrac{\rho Y_2}{M_2} + k_8 \, \dfrac{\rho Y_3}{M_3} \right)$

(e) $\quad R_7 = \dfrac{\rho Y_6 M_7}{M_6} \left(6 k_2 \dfrac{\rho Y_1}{M_1} + \dfrac{7}{2} k_5 \, \dfrac{\rho Y_2}{M_2} + k_8 \dfrac{\rho Y_3}{M_3} - 2 k_3 \, \rho Y_1 \dfrac{M_7}{M_1} \right)$

(f) $\quad R_8 = - \left(k_4 \, \rho Y_1 \dfrac{M_8}{M_1} + \dfrac{3}{4} k_7 \, \rho^2 \, \dfrac{Y_2 Y_8}{M_2} + \tfrac{1}{2} k_{10} \, \rho Y_3 \dfrac{M_8}{M_3} \right)$

(g) $\quad R_9 = 2 \, \rho Y_1 \dfrac{M_9}{M_1} \left(k_2 \dfrac{\rho Y_6}{M_6} + k_3 + k_4 \right) + \dfrac{3}{2} \, \rho Y_2 \dfrac{M_9}{M_2} \left(k_5 \dfrac{\rho Y_6}{M_6} + \right.$

$\qquad \left. k_7 \dfrac{\rho Y_8}{M_8} \right) + \rho Y_3 \, \dfrac{M_9}{M_3} \left(k_8 \dfrac{\rho Y_6}{M_6} + k_{10} \right)$

(h) $\quad R_4 = \rho Y_1 \dfrac{M_4}{M_1} \left(\tfrac{1}{2} k_1 + 2 k_3 + k_4 \right) + \tfrac{1}{2} k_7 \, \rho^2 Y_2 Y_8 \dfrac{M_4}{M_2 M_8}$